Green's functions for a face centered orthorhombic lattice*

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Diagonal and off-diagonal matrix elements of the Green's functions for a *face centered orthorhombic* lattice are presented in terms of integrals of complete elliptic integrals of the first and third kind. These Green's functions are also applicable to structures like that of the benzene crystal (space group D_{2h}^{15}, interchange symmetry D_2).

I. INTRODUCTION

Lattice Green's functions proved to be a powerful tool in the determination of impurity states in crystals. Considerable difficulties have been encountered in numerical calculations even for simple types of Green's function matrix elements.[1] Analytical expressions simplify the calculation of the Green's function matrix element, however these analytical expressions are only available for the simplest type crystal energy dispersion relations. Extensive use has been made of the complete elliptic integral of the first kind for the derivation of the diagonal matrix elements of the Green's function of square and rectangular lattices.[2,3] Green's function diagonal and off-diagonal matrix elements were given in terms of complete elliptic integrals of the first, second, and third kind by Hoshen and Jortner[4] for square lattices for the energy dispersion relation $2p\cos(x)+4q\cos(x/2)\cos(y/2)$, where p and q are intermolecular interaction parameters. Diagonal matrix elements of Green's functions for the three-dimensional cubic lattice can also be expressed in terms of integrals of complete elliptic integrals of the first kind.[5] Expressions for the Green's functions of products of complete elliptic integrals are available for fcc and bcc lattices.[3] Horiguchi, Yamazuki, and Morita[6] derived Green's function expressions for orthorhombic lattices in terms of complete elliptic integrals of the first kind. In Sec. II of this paper diagonal and off-diagonal matrix elements of the Green's function for face centered orthorhombic lattices will be presented. These matrix elements will be given in terms of integrals of complete elliptic integrals of the first and third kind. The expression derived in Sec. II will be applied in Sec. III for a numerical calculation of the Green's function matrix elements for some dispersion relations.

It should be noted that the lattice Green's function for the face centered orthorhombic Green's functions derived in this paper can be applied to benzene crystals belonging to the D_{2h}^{15} space group which contains four molecules per unit cell. The application of these Green's functions for isotopic impurity clusters in the benzene crystal will be given elsewhere.[7]

II. DERIVATIONS OF THE GREEN'S FUNCTIONS MATRIX ELEMENTS

In this section, expressions will be derived for the diagonal and three off-diagonal matrix elements of the Green's function for face centered orthorhombic crystals. The off-diagonal matrix elements correspond to the three nearest face centered neighbor molecules. The energy dispersion relation for this system is

$$h(x,y,z)=4A\cos x\cos y+4B\cos y\cos z+4C\cos z\cos x, \tag{1}$$

where

$$-\pi<x\leq\pi,\quad -\pi<y\leq\pi,\quad -\pi<z\leq\pi.$$

A, B, C are the interaction parameters between a molecule at the origin and the three face centered molecules, respectively.

The four Green's function matrix elements are given by

$$g_0(E)=\frac{1}{4\pi^3}\int_{-\pi/2}^{\pi/2}dy\int_{-\pi}^{\pi}dz\int_{-\pi}^{\pi}\frac{dx}{E-h(x,y,z)}, \tag{2}$$

$$g_1(E)=\frac{1}{4\pi^3}\int_{-\pi/2}^{\pi/2}dy\exp(iy)\int_{-\pi}^{\pi}dz\int_{-\pi}^{\pi}\frac{\exp(ix)\,dx}{E-h(x,y,z)}, \tag{3}$$

$$G_2(E)=\frac{1}{4\pi^3}\int_{-\pi/2}^{\pi/2}dy\exp(iy)\int_{-\pi}^{\pi}dz\exp(iz)\int_{-\pi}^{\pi}\frac{dx}{E-h(x,y,z)}, \tag{4}$$

$$g_3(E)=\frac{1}{4\pi^3}\int_{-\pi/2}^{\pi/2}dy\int_{-\pi}^{\pi}dz\exp(iz)\int_{-\pi}^{\pi}\frac{dx\exp(ix)}{E-h(x,y,z)}. \tag{5}$$

It should be noted that the integration limits over the y variable can be changed. Thus the following expression would hold for Eqs. (2)–(5):

$$2\int_{-\pi/2}^{\pi/2}dy\int_{-\pi}^{\pi}dz\int_{-\pi}^{\pi}dx\,F(x,y,z)=\int_{-\pi}^{\pi}dy\int_{-\pi}^{\pi}dz\int_{-\pi}^{\pi}dx\,F(x,y,z), \tag{6}$$

where $F(x,y,z)$ represents the integrands in Eq. (2)–(5).

Equation (2)–(5) can be recast in the following form:

$$g_0(E)=\frac{2}{\pi^2}\int_0^{\pi/2}dy\int_0^{\pi}dz\,I_0(y,z), \tag{7}$$

$$g_1(E)=\frac{2}{\pi^2}\int_0^{\pi/2}dy\cos y\int_0^{\pi}dz\,I_1(y,z), \tag{8}$$

$$g_2(E)=\frac{2}{\pi^2}\int_0^{\pi/2}dy\cos y\int_0^{\pi}dz\cos z\,I_0(y,z), \tag{9}$$

$$g_3(E)=\frac{2}{\pi^2}\int_0^{\pi/2}dy\int_0^{\pi}dz\cos z\,I_1(y,z), \tag{9'}$$

TABLE I. Setting signs for A, B, and C.

Given B, C*		Setting signs for: A	B	C
$B>0$,	$C>0$	A	B	C
$B>0$,	$C<0$	$-A$	B	$-C$
$B<0$,	$C>0$	$-A$	$-B$	C
$B<0$,	$C<0$	A	$-B$	$-C$

*The sign of A can be either positive or negative.

where

$$I_n(y,z) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{dx\,\exp(inx)}{E - 4(A\cos x\cos y + B\cos y\cos z + C\cos x\cos z)}, \tag{10}$$

and $n=0,1$.

The integral I_n can be easily evaluated by a complex contour integration. When the density of state function for the energy dispersion Eq. (1) is nonzero, $I_n(y,z)$ should be treated as a special case. In this case E is substituted by $E-i\epsilon$, where ϵ is a small positive number. ϵ is set to zero when the limit of $I_n(y,z)$ is taken.

Substituting $u=\exp(ix)$ in Eq. (10) and integrating over the unit circle in the complex u plane we obtain

$$I_n(y,z) = \lim_{\epsilon\to+0} \frac{i}{\pi}\oint \frac{u^n\,du}{xu^2 - 2(E - i\epsilon - \mu)u + \chi}, \tag{11}$$

where

$$\chi = 4(A\cos y + C\cos z),$$

$$\mu = 4B\cos y\cos z.$$

$I_n(y,z)$ has a real value for

$$(E-\mu)^2 \geqslant \chi^2 \tag{12}$$

and is given by

$$I_n(y,z) = \xi u^m/\Delta', \tag{13}$$

where

$\xi = 1$ and $u_m = u^-$ for $E>\mu$,

$\xi = -1$ and $u_m = u^+$ for $E<\mu$.

Δ' is given by

$$\Delta' = \lim_{\epsilon\to+0}[(E - i\epsilon - \mu)^2 - \chi)]^{1/2}. \tag{14}$$

$u^{\pm}$ are represented by:

$$u^{\pm} = \lim_{\epsilon\to+0} \frac{E - i\epsilon - \mu \pm \Delta'}{\chi}. \tag{15}$$

It should be noted that for the case represented by Eq. (12) it is immaterial whether the limits are taken before or after the integration of Eq. (11), since we deal with two poles, neither one of which is located on the unit circle for $\epsilon\to+0$.

The situation is different for

$$(E-\mu)^2 < \chi^2. \tag{16}$$

The two roots $u^{\pm}$ lie on the unit circle for which $\epsilon\to+0$, so that the limit is determined after the residues of Eq. (11) are calculated. The limiting process is described in Appendix A. The complex integral $I_n(y,z)$ is given for this case by:

$$I_n(y,z) = \xi u^+/\Delta', \tag{17}$$

where $\xi=-1$, and u^+ and Δ' are given by Eqs. (15) and (14), respectively. Hence for the complex I_n, ξ is independent of y and z.

At this point it becomes necessary to assume certain relationships between the interaction parameters, A, B, and C. Without loss of generality we can assume $|C|>|B|>|A|$. This can be done because the dispersion relation (1) is symmetrical with respect to x, y, and z. In addition, we may assume that $C>0$ and $B>0$. When B or C (or both) are negative they can be set positive according to Table I. This setting leaves the Green's functions invariant.

Equations (7)–(10) can be recast in the form

$$g_0(E) = \frac{2}{\pi^2}\int_0^{\pi/2} dy \int_0^{\pi} \frac{\xi\,dz}{\Delta'}, \tag{18}$$

$$\begin{aligned} g_1(E) &= \frac{2}{\pi^2}\int_0^{\pi/2} dy\cos y \int_0^{\pi} \frac{\xi(E-\mu)\,dz}{\chi\Delta'} - \frac{2}{\pi^2}\int_0^{\pi/2} dy\cos y\int_0^{\pi}\frac{dz}{4(A\cos y + C\cos z)} \\ &= \frac{2}{\pi^2}\int_0^{\pi/2} dy\cos y\int_0^{\pi}\frac{\xi(E - 4B\cos y\cos z)\,dz}{4(A\cos y + C\cos z)\Delta'}, \end{aligned} \tag{19}$$

$$g_2(E) = \frac{2}{\pi^2}\int_0^{\pi/2} dy\cos y \int_0^{\pi} \frac{\xi\cos z\,dz}{\Delta'}, \tag{20}$$

$$\begin{aligned} g_3(E) &= \frac{2}{\pi^2}\int_0^{\pi/2} dy \int_0^{\pi} \frac{\xi\cos z(E-\mu)\,dz}{\chi\Delta'} - \frac{2}{\pi^2}\int_0^{\pi/2} dy\int_0^{\pi}\frac{\cos z\,dz}{4(A\cos y + C\cos z)} \\ &= \frac{E}{4C}g_0(E) - \frac{A}{C}g_1(E) - \frac{B}{C}g_2(E) - \frac{1}{4C}. \end{aligned} \tag{21}$$

The Green's functions matrix elements, Eqs. (18)–(21) are real for the inequality Eq. (12) and complex for the inequality Eq. (16). $g_3(E)$ is given in terms of $g_0(E)$, $g_1(E)$, and $g_2(E)$. Thus we shall limit the discussion only to those three Green's functions matrix elements.

Substituting $t=\cos z$ in Eqs. (18)–(21), the $g_i(E)$ functions, $i=0,1,2$, can be expressed in the form

$$g_i(E) = \int_0^{\pi/2} H_i(y)\,dy, \tag{22}$$

where

$$H_i(y) = \int_{-1}^{1} u_i(t)\,dt \tag{23}$$

and the $u_i(t)$ are given by

$$u_0(t) = \frac{2\xi}{\pi^2\Delta}, \tag{24}$$

$$u_1(t) = \frac{2B(\cos^2 y)\xi(p_1 - t)}{\pi^2 C(p-t)\Delta}, \tag{25}$$

$$u_2(t) = \frac{2(\cos y)\xi t}{\pi^2\Delta}, \tag{26}$$

TABLE II. Boundaries for $\mathcal{R}$.

Boundary \ Condition	$A<0$, $C>B-A$ Case (i)	$A<0$, $C<B-A$ Case (ii)	$A>0$, $C>B+A$ Case (iii)	$A>0$, $C<A+B$ Case (iv)
A_1	$4(A-B-C)$	$4(A-B-C)$	$4(A-B-C)$	$4(A-B-C)$
A_2	$-4C$	$-4C$	$-4C$	$-4C$
A_3	$4(B-C-A)$	0	$4(B-A-C)$	$4(B-A-C)$
A_4	0	$4(B-C-A)$	$-4AB/C$	$-4AB/C$
A_5	$-4AB/C$	$-4AB/C$	0	$4(C-A-B)$
A_6	$4(C-A-B)$	$4(C-A-B)$	$4(C-A-B)$	0
A_7	$4C$	$4C$	$4C$	$4C$
A_8	$4(A+B+C)$	$4(C+A+B)$	$4(C+A+B)$	$4(C+B+A)$

where

$$p=-A\cos y/C,\quad p_1=E/4B\cos y,$$

$$\Delta=[16(C^2-B^2\cos^2 y)(t-1)(t+1)(t-\gamma)(t-\delta)]^{1/2}, \tag{27}$$

and γ and δ are

$$\gamma=\frac{E+4A\cos y}{4B\cos y-4C}, \tag{28}$$

$$\delta=\frac{E-4A\cos y}{4B\cos y+4C}. \tag{29}$$

The following relationships hold for γ and δ: When $E>r$ then $\delta>\gamma$, when $E<r$ then $\gamma>\delta$, where

$$r=-4AB\cos^2 y/C. \tag{30}$$

By utilizing Eqs. (28)–(30), it can be shown that for the real part of $g_i(E)$ ξ is independent of z, and depends only on y and is given by

$$\xi=\operatorname{sgn}(E-r). \tag{31}$$

The integrals over y of Eq. (22) take different forms in each of the nine $\mathcal{R}_i$ energy regions. The $\mathcal{R}_i$ regions for $i=2,3,\ldots,8$ are defined by $A_i>E>A_{i-1}$, $\mathcal{R}_1$ is defined by $E<A_1$ and $\mathcal{R}_9$ is defined by $E>A_8$. The A_i are the boundaries of these regions. There are four cases for these boundaries, and they are specified in Table II.

The $g_i(E)$ can be represented in term of the integrals $V_i(y_1,y_2)$, where the V_i are defined by:

$$V_i^{(l)}(y_s,y_j)=\int_{y_s}^{y_j}H_i^{(l)}(y)\,dy \tag{32}$$

where

$$0<y_s<y_j\leq\pi/2.$$

The index l denotes six energy regions $\mathcal{S}_l$, specified in Table III, for which $H_i(y)$ assumes a different form for each of the six regions. Hence Eqs. (22) are given as follows:

For the $\mathcal{R}_1$ Cases: (i), (ii), (iii), (iv),

$$g_i(E)=V_i^{(6)}(0,\pi/2). \tag{33}$$

For the $\mathcal{R}_2$ Cases: (i), (ii), (iii), (iv),

$$g_i(E)=V_i^{(5)}(0,y_1)+V_i^{(6)}(y_1,\pi/2). \tag{34}$$

For the $\mathcal{R}_3$ Cases: (i), (ii), (iii), (iv),

$$g_i(E)=V_i^{(5)}(0,y_2)+V_i^{(4)}(y_2,\pi/2). \tag{35}$$

For the $\mathcal{R}_4$ Cases: (i), (iii), (iv),

$$g_i(E)=V_i^{(4)}(0,\pi/2). \tag{36a}$$

For the $\mathcal{R}_4$ Case: (ii),

$$g_i(E)=V_i^{(5)}(0,y_2)+V_i^{(4)}(y_2,y_3)+V_i^{(3)}(y_3,\pi/2). \tag{36b}$$

For the $\mathcal{R}_5$ Cases: (iii) and (iv),

$$g_i(E)=V_i^{(3)}(0,y_3)+V_i^{(4)}(y_3,\pi/2). \tag{37a}$$

For the $\mathcal{R}_5$ Cases: (i) and (ii),

$$g_i(E)=V^{(4)}(0,y_3)+V^{(3)}(y_3,\pi/2). \tag{37b}$$

For the $\mathcal{R}_6$ Cases: (i), (ii), and (iii),

$$g_i(E)=V_i^{(3)}(0,\pi/2). \tag{38a}$$

For the $\mathcal{R}_6$ Case: (iv),

$$g_i(E)=V_i^{(2)}(0,y_4)+V_i^{(3)}(y_4,y_3)+V_i^{(4)}(y_3,\pi/2). \tag{38b}$$

For the $\mathcal{R}_7$ Cases: (i), (ii), (iii), and (iv),

$$g_i(E)=V_i^{(2)}(0,y_4)+V_i^{(3)}(y_4,\pi/2). \tag{39}$$

For the $\mathcal{R}_8$ Cases: (i), (ii), (iii), (iv),

$$g_i(E)=V_i^{(2)}(0,y_5)+V_i^{(1)}(y_5,\pi/2). \tag{40}$$

For the $\mathcal{R}_9$ Cases: (i), (ii), (iii), (iv),

$$g_i(E)=V_i^{(1)}(0,\pi/2). \tag{41}$$

The y_1, y_2, y_3, y_4, and y_5 are

$$y_1=\arccos\frac{E+4C}{4A-4B}, \tag{42a}$$

$$y_2=\arccos\frac{E+4C}{4B-4A}, \tag{42b}$$

TABLE III. The $\mathcal{S}_i$ regions.

$\mathcal{S}_l$ regions	Definition of energy regions*	Relationships for γ and δ
$\mathcal{S}_1$	$E>a$	$\delta>1;\ -1>\gamma$
$\mathcal{S}_2$	$a>E>b$	$1>\delta>-1>\gamma$
$\mathcal{S}_3$	$b>E>r$	$1>\delta>\gamma>-1$
$\mathcal{S}_4$	$r>E>c$	$1>\gamma>\delta>-1$
$\mathcal{S}_5$	$c>E>d$	$\gamma>1>\delta>-1$
$\mathcal{S}_6$	$E<d$	$\gamma>1;\ -1>\delta$

*$a=4(A+B)\cos y+4C$; $b=-4(A+B)\cos y+4C$; $c=4(B-A)\cos y-4C$; $d=4(A-B)\cos y-4C$; $r=-4AB\cos^2 y/C$; $a>b>r>c>d$.

TABLE IV. The Y parameters of Eqs. (57) and (58).

$\mathcal{S}_l$ regions	Y Real part	Y Imaginary part Range 1	Range 2
1	1	-1	-1
2	1	$-\delta$	-1
3	$-\gamma$	$-\gamma^{\dagger}$	$-\delta^{\dagger}$
4	$-\delta$	$-\delta^{\ddagger}$	$-\gamma^{\ddagger}$
5	$-\delta$	$-\delta$	-1
6	1	-1	-1

†,‡see the footnotes to Table V.

$$y_3 = \arccos\left(\frac{-EC}{4AB}\right)^{1/2}, \tag{42c}$$

$$y_3 = \arccos\frac{4C-E}{4A+4B}, \tag{42d}$$

$$y_5 = \arccos\frac{E-4C}{4A+4B}. \tag{42e}$$

It should be noted that $V_i^{(1)}(y_k, y_j)$ and $V_i^{(6)}(y_k, y_j)$ are real and have no imaginary component.

In order to carry the integration of Eq. (23) for $H_i(y)$ [or rather $H_i^{(l)}(y)$], we have to separate the real and imaginary parts of $H_i(y)$. This can be done by defining $u_i''(t)$ functions, where:

$$u_0''(t) = \frac{2}{\pi^2\Delta''}, \tag{43}$$

$$u_1''(t) = \frac{-2B\cos^2 y(p_1 - t)}{\pi^2 C(p-t)\Delta''}, \tag{44}$$

$$u_2''(t) = \frac{2t\cos y}{\pi^2\Delta''}, \tag{45}$$

where Δ'' is given by

$$\Delta'' = [16(C^2 - B^2\cos^2 y)(t-1)(t+1)(t-\gamma)(\delta - t)]^{1/2}$$
$$= i\Delta \tag{46}$$

and Δ was given by Eq. (27).

The following relation holds between $u_i''(t)$, Eqs. (43)–(45) and $u_i(t)$, Eqs. (24)–(26), for the imaginary part of the Green's functions:

$$u_i''(t) = -iu_i(t). \tag{47}$$

Let us define two auxiliary functions $W(t_1, t_2)$ and $W''(t_1, t_2)$:

$$W_i(t_1, t_2) = \int_{t_1}^{t_2} u_i(t)\,dt \tag{48}$$

and

$$W_i''(t_1, t_2) = \int_{t_1}^{t_2} u_i''(t)\,dt, \tag{49}$$

where $t_2 > t_1$, $t_1 = -1, \gamma, \delta$, and $t_2 = \gamma, \delta, 1$. The $H_i^{(l)}(y)$ are given for each of the $\mathcal{S}_l$ regions in the form

$$H_i^{(1)}(y) = W_i(-1, 1), \tag{50}$$

$$H_i^{(2)}(y) = W_i(-1, \delta) + iW''(\delta, 1), \tag{51}$$

$$H_i^{(3)}(y) = W_i(\gamma, \delta) + i[W_i''(-1, \gamma) + W_i''(\delta, 1)], \tag{52}$$

$$H_i^{(4)}(y) = W_i(\delta, \gamma) + i[W_i''(-1, \delta) + W_i''(\gamma, 1)], \tag{53}$$

$$H_i^{(5)}(y) = W_i(\delta, 1) + iW_i''(-1, \delta), \tag{54}$$

$$H_i^{(6)}(y) = W_i(-1, 1). \tag{55}$$

The W_i and W_i'' functions can be expressed in terms of complete elliptic integrals of the first and third kind,[8] and are given by

$$W_0'(t_1, t_2) = \xi_l fK(k), \tag{56}$$

$$W_1'(t_1, t_2) = -\xi_l f\frac{B\cos^2 y(p_1 + Y)}{C(p+Y)}\,T(k, \alpha_4^2, \alpha_3^2), \tag{57}$$

$$W_2'(t_1, t_2) = -\xi_l f\cos y\,Y\,T(k, \alpha_1^2, \alpha_2^2), \tag{58}$$

where W_i' represents either W_i or W_i''.

For $W_i'' = W_i'$, $\xi_l = 1$; and for $W_i = W_i'$, $\xi_l = 1$ in the regions $\mathcal{S}_1$, $\mathcal{S}_2$, $\mathcal{S}_3$, but $\xi_l = -1$ for the regions $\mathcal{S}_4$, $\mathcal{S}_5$, $\mathcal{S}_6$ (see Table III). The parameter Y in Eqs. (57) and (58) is given in Table IV. $K(k)$ in Eq. (56) denotes a complete elliptic integral of the first kind with a modulus k. The T functions in Eqs. (57) and (58) are given in the form[8]

$$T(k, \alpha^2, \beta^2) = (1/\alpha^2)[(\alpha^2 - \beta^2)\Pi(k, \alpha^2) + \beta^2 K(k)]. \tag{59}$$

TABLE V. Parameters for the imaginary parts of the Green's functions.

$\mathcal{S}_l$ region	k'^2	Range	α_1^2	α_2^2	α_3^2	α_4^2
2	$\frac{V^2-\epsilon_m}{8q}$		$\frac{(1-\delta)}{2}$	$\frac{(\delta-1)}{2\delta}$	$\frac{(1-\delta)(p_1+1)}{2(p_1+\delta)}$	$\frac{(1-\delta)(p_1+1)}{2(p_1+\delta)}$
3	$\frac{\epsilon_m-V}{\epsilon_p-W}$	† 1	$\frac{\gamma+1}{\delta+1}$	$\frac{\delta(\gamma+1)}{\gamma(\delta+1)}$	$\frac{(p_1-\delta)(\gamma+1)}{(p_1-\gamma)(\delta+1)}$	$\frac{(p-\delta)(\delta+1)}{(p-\gamma)(\gamma+1)}$
		2	$\frac{1-\delta}{1-\gamma}$	$\frac{\gamma(1-\delta)}{\delta(1-\gamma)}$	$\frac{(p_1-\gamma)(1-\delta)}{(p_1-\delta)(1-\gamma)}$	$\frac{(p-\gamma)(1-\delta)}{(p-\delta)(1-\gamma)}$
4	$\frac{\epsilon_p-W}{\epsilon_m-V}$	‡ 1	$\frac{\delta+1}{\gamma+1}$	$\frac{\gamma(\delta+1)}{\delta(\gamma+1)}$	$\frac{(p_1-\gamma)(\delta+1)}{(p_1-\delta)(\gamma+1)}$	$\frac{(p-\gamma)(\delta+1)}{(p-\delta)(\gamma+1)}$
		2	$\frac{1-\gamma}{1-\delta}$	$\frac{\delta(1-\gamma)}{\gamma(1-\delta)}$	$\frac{(p_1-\delta)(1-\gamma)}{(p_1-\gamma)(1-\delta)}$	$\frac{(p-\delta)(1-\gamma)}{(p-\gamma)(1-\delta)}$
5	$\frac{\epsilon_p-W}{8q}$		$\frac{\delta+1}{2}$	$\frac{\delta+1}{2\delta}$	$\frac{(\delta+1)(p_1-1)}{2(p_1-\delta)}$	$\frac{(\delta+1)(p-1)}{2(p-\delta)}$

†(1) parameters for $W_i''(-1,\gamma)$; (2) parameters for $W_i''(\delta,1)$ (see Eq. 52).

‡(1) parameters for $W_i''(-1,\delta)$; (2) parameters for $W_i''(\gamma,1)$ (see Eq. 53). V, W, ϵ_m, ϵ_p, q are defined in the footnote to Table VI.

TABLE VI. Parameters for the real part of the Green's functions.

$\mathcal{S}_I$ region	f	k^2	α_1^2	α_2^2	α_3^2	α_4^2
1	$\frac{4}{\pi^2(\epsilon_p - W)^{1/2}}$	$\frac{8q}{\epsilon_p - W}$	$\frac{2}{1-\gamma}$	$\frac{2}{\gamma-1}$	$\frac{2(p_1-\gamma)}{(1-\gamma)(p_1+1)}$	$\frac{2(p-\gamma)}{(1-\gamma)(p+1)}$
2	$\frac{1}{\pi^2}\left(\frac{2}{q}\right)^{1/2}$	$\frac{\epsilon_p - W}{8q}$	$\frac{\delta+1}{\delta-\gamma}$	$\frac{\gamma(\delta+1)}{\gamma-\delta}$	$\frac{(\delta+1)(p_1-\gamma)}{(\delta-\gamma)(p_1+1)}$	$\frac{(\delta+1)(p-\gamma)}{(\delta-\gamma)(p+1)}$
3	$\frac{4}{\pi^2(\epsilon_p - W)^{1/2}}$	$\frac{8q}{\epsilon_p - W}$	$\frac{\delta-\gamma}{\delta+1}$	$\frac{\gamma-\delta}{\gamma(\delta+1)}$	$\frac{(\delta-\gamma)(p_1+1)}{(\delta+1)(p_1-\gamma)}$	$\frac{(\delta-\gamma)(p+1)}{(\delta+1)(p-\gamma)}$
4	$\frac{4}{\pi^2(\epsilon_m - V)^{1/2}}$	$\frac{8q}{V-\epsilon_m}$	$\frac{\gamma-\delta}{\gamma+1}$	$\frac{\delta-\gamma}{\delta(\gamma+1)}$	$\frac{(\gamma-\delta)(p_1+1)}{(\gamma+1)(p_1-\delta)}$	$\frac{(\gamma-\delta)(p+1)}{(\gamma+1)(p-\delta)}$
5	$\frac{1}{\pi^2}\left(\frac{-2}{q}\right)^{1/2}$	$\frac{V-\epsilon_m}{8q}$	$\frac{1-\delta}{2}$	$\frac{(\delta-1)}{2}$	$\frac{(1-\delta)(p_1+1)}{2(p_1-\delta)}$	$\frac{(1-\delta)(p+1)}{2(p-\delta)}$
6	$\frac{4}{\pi^2(\epsilon_m - V)^{1/2}}$	$\frac{8q}{V-\epsilon_m}$	$\frac{2}{1-\delta}$	$\frac{2\delta}{\delta-1}$	$\frac{2(p_1-\delta)}{(1-\delta)(p_1+1)}$	$\frac{2(p-\delta)}{(1-\delta)(p+1)}$

$V=16(A+B)^2\cos^2y$, $W=16(A-B)^2\cos^2y$, $q=8AB\cos^2y+2CE$, $\epsilon_m=(E-4C)^2$, $\epsilon_p=(E+4C)^2$. $\epsilon_m=(E-4C)^2$, $\epsilon_p=(E+4C)^2$.

The modulus k, and the parameters α_1^2, α_2^2, α_3^2, and α_4^2 and f are given for W_i in Table VI and for W_i'' in Table V. Π denotes a complete elliptic integral of the third kind. It should be noted that the modulus k of W_i'' is the complementary modulus k' of W_i.

The following relationships hold for the parameters of $\Pi(k, \alpha^2)$ for W_1 and W_2 (real case):

$$0 < \alpha_1^2 < k^2, \tag{60}$$

$$\alpha_4^2 > 1. \tag{61}$$

This is known as the hyperbolic case for Π, where Π can be given in terms of the Jacobian zeta function Z.

The relationships for the parameters of $\Pi(k, \alpha^2)$ for W_i'' and W_2'' are (imaginary case)

$$k^2 < \alpha_1^2 < 1, \tag{62}$$

$$\alpha_4^2 < 0. \tag{63}$$

This is known as the circular case for Π, where Π can be given in terms of the Heuman lambda function Λ_0.

III. NUMERICAL CALCULATIONS

The Green's function matrix elements g_0, g_1, and g_2 can be evaluated utilizing the integration formulas Eqs. (33)–(41). $g_3(E)$ can be simply determined from Eq. (21), after g_0, g_1, and g_2 are evaluated. The integrations Eqs. (33)–(41) as defined in Eq. (32) can be determined numerically. There are no available analytical expressions for these integrals. The integrand of Eq. (32), $H_i^{(l)}$ includes both a real and an imaginary component for $l=2,3,4,5$ (see Table III). The $H_i^{(l)}$ functions are defined by Eqs. (50)–(55) in terms of the W_i and W_i'' functions. The W_i and W'' functions are given in terms of complete elliptic integrals of the first and third kind [see Eqs. (56)–(59)]. The various parameters of Eqs. (56)–(59) are displayed in Tables IV, V, and VI. The complete elliptic integrals of the third kind can be given in terms of Z or Λ_0 functions.[8] The Z and Λ_0 functions can be represented in terms of both complete elliptic integrals of the first and second kind, and incomplete elliptic integrals of the first and second kind. All these complete and incomplete elliptic integrals can be calculated utilizing standard computer programs.[9]

The integrations in Eqs. (33)–(41) are somewhat complicated due to the existence of a logarithmic singularity in $K(k)$ for $k=1$. However, the singularity will be located at one of the integration limits of Eq. (32), when they occur. To avoid the singularities, a Gauss quadrature was applied for the numerical integrations of Eqs. (33)–(41). It was determined that the singularities do not have a significant effect on the calculations. This effect was explored by removing the singularity from the integrand of Eq. (32) for W_0'' and W_0. An example of such a process is given in Appendix B. It was found that the singularities could be safely ignored, since removal of the singularities changed the final results by 0.1% at most.

Results for the computation of the $g_0(E)$, $g_1(E)$, $g_2(E)$, and $g_3(E)$ are given in Figs. 1 and 2 for the real and imaginary parts of the Green's function. The A, B, and C parameters in Fig. 1 are taken from Kopelman and Laufer,[10] corresponding to case (iii) whereas the parameters in Fig. 2 are arbitrary, and correspond to case (iv).

A specific example for determining a Green's function matrix element is given in Appendix C. The complete program for calculating the Green's function matrix elements for the various A, B, and C interaction parameters has been coded in FORTRAN, and is available upon request from the authors of this paper.

APPENDIX A

Utilizing a binomial expansion of the radical Δ' of Eq. (14), and returning the term linear in ϵ we obtain for the complex case of Eq. (15)

$$u^{\pm}=\frac{1}{\chi}\left\{E-i\epsilon-\mu\pm i(\chi^2-(E-\mu)^2)^{1/2}\left(1+\frac{i\epsilon(E-\mu)}{\chi^2-(E-\mu)^2}\right)\right\}$$
$$=\frac{1}{\chi}\left\{[E-\mu\pm i(\chi^2-(E-\mu)^2)^{1/2}]\left(1\pm\frac{\epsilon}{(\chi^2-(E-\mu)^2)^{1/2}}\right)\right\}. \tag{A1}$$

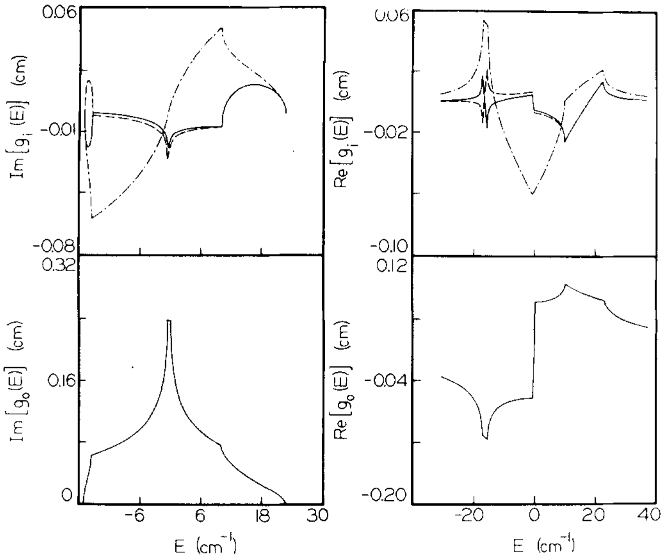

FIG. 1. Real and imaginary parts of the Green's functions matrix element $g_i(E)$. Bottom figures denote diagonal element $g_0(E)$. Top figures denote off-diagonal elements $g_i(E)$: --- $g_1(E)$, —$g_2(E)$, — - —$g_3(E)$ for interaction parameters $A = 0.7$ cm^{-1}, $B = 0.9$ cm^{-1}, $C = 4.1$ cm^{-1} (see Eq. 1).

To determine whether u^+ or u^- lies within the unit circle the absolute value of the poles is taken:

$$|u^\pm| = \left|\frac{E-\mu \pm i\chi^2-(E-\mu)^2}{\chi}\right| \left|1 \mp \frac{\epsilon}{(\chi^2-(E-\mu))^{1/2}}\right|$$

$$= 1 \cdot \left|1 \mp \frac{\epsilon}{(\chi^2-(E-\mu)^2)^{1/2}}\right|. \qquad \text{(A2)}$$

Since ϵ is a positive number, $|u^+| < 0$ and $|u^-| > 0$. Hence $|u^+|$ lies within the unit circle and contributes to the residue.

It should be noted that the choice of ϵ to be positive is required by the physical situation. The density of states function $\rho(E)$ given by[1]

$$\rho(E) = \frac{1}{\pi}\,\mathrm{Im}\,g_0(E) \qquad \text{(A3)}$$

must be positive. If ϵ is taken to be negative, u^- would lie within the unit circle, and the $\rho(E)$ would be negative.

APPENDIX B

The effect of the singularities of the integral given by Eq. (32), can be best illustrated by treating an example of such an integral. Let us look at the imaginary part of Eq. (37a) for $i = 0$,

$$\mathrm{Im}\,g_0(E) = \mathrm{Im}\,V_0^{(3)}(0, y_3) + \mathrm{Im}\,V_0^{(4)}(y_3, \pi/2)$$
$$= \int_0^{y_3} f_3 K(k_3)\,dy + \int_{y_3}^{\pi/2} f_4 K(k_4)\,dy, \qquad \text{(B1)}$$

f_3 and f_4 denote the f parameters for regions S_3 and S_4, respectively. The values of f_3 and f_4 are given in Table V. For $y = y_3$ we shall define f':

$$f' = f_3 = f_4. \qquad \text{(B2)}$$

The moduli k_3 and k_4 are given by Table VI and for $y = y_3$ both approach the value of one.

Utilizing the limit[1]

$$\lim_{k\to 1} K(k) = \ln\frac{4}{k'}, \qquad \text{(B3)}$$

we obtain for Eq. (B1),

$$\mathrm{Im}\,g_0(E) = \int_0^{y_3}[f_3K(k_3) - f'\ln(-q)]\,dy$$
$$+ \int_{y_3}^{\pi/2}[f_4K(k_4) - f'\ln q]\,dy + f'\int_0^{\pi/2}\ln|q|\,dy, \qquad \text{(B4)}$$

where q is given in Table VI.

For the limits

$$\lim_{y\to y_3} k_3 = \lim_{y\to y_3} k_4 = 1, \qquad \text{(B5)}$$

the following expressions are obtained:

$$\lim_{y\to y_3}[f_3K(k_3) - f'\ln(-q)] = \lim_{y\to y_3}[f_4K(k_4) - f'\ln q] = 0. \qquad \text{(B6)}$$

By utilizing Eq. (B6), we may observe that the singularities have been removed from the first two integrals of Eq. (B4). The singularity exists only for the integral $J_1 = \int_0^{\pi/2}\ln|q|\,dy$. However, this integral has an analytical expression

$$= (\pi/2)k\,|2CE| + \int_0^{\pi/2}\ln|1 + p_2\cos^2 y|, \qquad \text{(B7)}$$

where p_2 is given by

$$p_2 = 4AB/CE.$$

The integral

$$J_2 = \int_0^{\pi/2}\ln|1 + p_2\cos^2 y|\,dy \qquad \text{(B8)}$$

is given by

$$J_2 = \pi\ln\left(\frac{1 + (1 + p_2)^{1/2}}{2}\right). \qquad \text{(B9)}$$

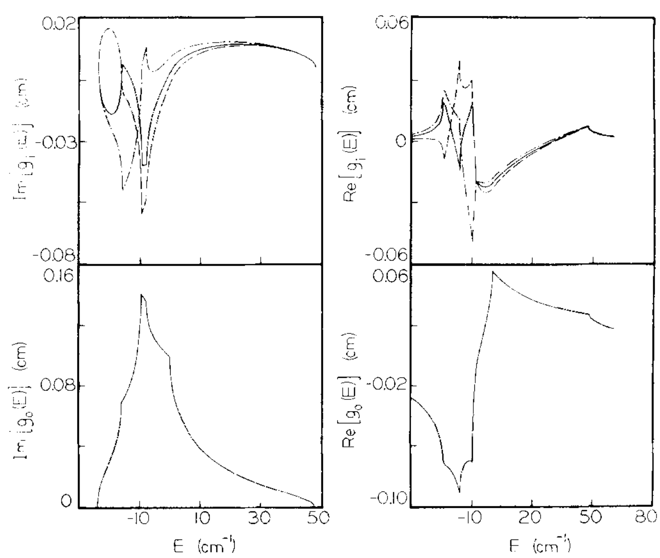

FIG. 2. Real and imaginary parts of the Green's function matrix elements $g_i(E)$ [for notations see footnotes to Fig. 1] for interaction parameters $A = 2$ cm^{-1}, $B = 3$ cm^{-1}, and $C = 4$ cm^{-1}.

APPENDIX C

The representation of the Green's function matrix elements $q_i(E)$ for the crystal structure and interactions, under consideration, are numerous and complex. These representations change with the relative magnitude of the interaction parameters A, B, and C, as well as the interactions signs, and energy value E. A specific example for determining the appropriate representation, using the prescription given above would be illustrative.

We shall assume $A=2$, $B=3$, $C=4$, and that we are looking for the imaginary part of $q_2(E)$, where $E=-10$ (see Fig. 2). In order to elucidate the form of $\operatorname{Im} g_2(E)$, we shall envoke the following steps:

(a) Utilizing Table I, we observe that the signs of A, B, and C remain unchanged, because $B>0$, and $C>0$.

(b) Inspecting Table II, we find that Case (iv) is applicable for our parameter set, and that $A_3 < E < A_4$, implying $E \in \mathcal{R}_4$.

(c) The Green's function matrix element $\operatorname{Im} g_2(E)$, which corresponds to Case (iv) and region $\mathcal{R}_4$, is given by Eq. (36a). Hence,

$$\operatorname{Im} g_2(E) = \operatorname{Im} V_2^{(4)}(0, \pi/2) = \int_0^{\pi/2} \operatorname{Im} H_2^{(4)}(y)\, dy. \qquad \text{(C1)}$$

(d) The superscript (4) in $H_2^{(4)}$ of Eq. (C1) denotes energy region $\mathcal{S}_4$, defined in Table III. $\operatorname{Im} H_2^{(4)}(E)$ is expressed by the auxiliary function W_2'' given by Eq. (53). Taking the imaginary part of Eq. (53), we obtain for Eq. (C1):

$$\operatorname{Im} g_2(E) = \int_0^{\pi/2} W_2''(-1, \delta)\, dy + \int_0^{\pi/2} W_2''(\gamma, 1)\, dy, \qquad \text{(C2)}$$

where γ and δ are given by Eqs. (28) and (29), respectively.

(e) The W_2'' functions are given by Eq. (58) for which $\xi_l = 1$. Thus, the W_2'' functions given by Eq. (C2) can be represented in the form:

$$W_2''(t_1, t_2) = f Y \alpha_1^{-2}[(\alpha_1^2 - \alpha_2^2)\Pi(k', \alpha_1^2) + \alpha_1^2 K(k')] \cos y. \qquad \text{(C3)}$$

The parameters f and $(k')^2$, for the region $\mathcal{S}_4$, are displayed in Tables VI and V, respectively. Similarly, the parameters α_1^2 and α_2^2 of Eq. (C3), for range (1) of region $\mathcal{S}_4$, corresponding to the function $W''(-1, \delta)$, and for range (2) to the function $W''(1, \gamma)$, are given in Table V. The Y parameters for ranges (1) and (2) of region $\mathcal{S}_4$ are given in Table IV.

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